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Mixed finite element discretization of a model for organic pollution in waters

Part I. The problem and its discretization

Faker Ben Belgacem¹, Christine Bernardi², Frédéric Hecht³, and Stéphanie Salmon⁴

Abstract

We consider a mixed reaction diffusion system describing the organic pollution in stream-waters. It may be viewed as the static version of Streeter–Phelps equations relating the Biochemical Oxygen Demand and Dissolved Oxygen to which dispersion terms are added. In this work, we propose a mixed variational formulation and prove its well-posedness. Next, we develop two finite element discretizations of this problem and establish optimal a priori error estimates for the second discrete problem.

Résumé

Nous nous intéressons à un système d'équations aux dérivées partielles qui modélise la pollution organique dans des rivières et nous prouvons qu'il est bien posé. Puis nous proposons deux discrétisations par éléments finis de ce problème et démontrons pour la seconde des estimations a priori optimales de l'erreur.

Key words: Variational formulation, non-symmetric mixed problem, mixed finite elements, generalized saddle point theory, organic pollution.

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1 Introduction

Since the early (advection-)reaction formulation written by Streeter and Phelps in 1925 to study the Ohio river (see [22]), sophisticated modeling of the organic pollution in stream-waters has been elaborated. Taylor's dispersion is particularly incorporated that bring substantial difficulties in the mathematical study. Readers interested in are referred to [20, 11, 21] for the dispersion-reaction models so as more complete (non-linear) ones. The central element of such problems is the oxygen. The main tracers currently used are the density b of the Biochemical Oxygen Demand (BOD) and the concentration c of the Dissolved Oxygen (DO). In the steady state, they are solutions of the reaction-dispersion equations, in a bounded two or three-dimensional domain Ω ,

$$\begin{aligned} -\operatorname{div}(d\nabla b) + r b &= f && \text{in } \Omega, \\ -\operatorname{div}(d\nabla c) + r_* c + r b &= g && \text{in } \Omega, \\ c &= \alpha && \text{on } \partial\Omega, \\ d\partial_n c &= \beta && \text{on } \partial\Omega. \end{aligned} \tag{1.1}$$

The symbol d is the dispersion coefficient and (r, r_*) are reaction parameters. They are all space-varying. The BOD is the amount of oxygen per unit volume, necessary for the micro-organisms and aerobic bacteria to break down the organic matter contained in the water. The DO is the oxygen concentration housed in a unit volume of water. The right-hand side f in (1.1), describes the source of the pollution, while the datum g can be for instance the uptake oxygen from the atmosphere to reduce the deficit of oxygen caused by the biodegradation of the organic pollutants. Some authors favor the oxygen deficit density which is the gap between the saturation oxygen level and the actual dissolved oxygen content. The coupling term represented by $r b$ in the second equation is the depletion of oxygen due to elevated BOD. The boundary data (α, β) are the measures of the DO and its flux at the boundary. Currently, no oxygen flux is generated by the environmental medium so that β is very near zero.

Differential system (1.1) is the steady form of the full time-dependent BOD/DO model, set in two- or three-dimensional body of water such as a lake, a lagoon or an estuary. It is actually obtained by adding to the elementary Streeter–Phelps differential equation the dispersion term. Solving the steady problem may have its own interest, the related problem aims the reconstruction of some polluting flux $d\partial_n b$, through the boundary $\partial\Omega$, caused by many factor such as domestic, agricultural or breeding activities. The lack of boundary data on b is balanced by two conditions on the dissolved oxygen c . Indeed, measurements on c are easy and instantaneously obtained while those on b need conducting a strict chemical protocol and last five days. Note that we do not include the advection in our model. Nevertheless, the study conducted here extends as well to that case.

Deriving theoretical results for the steady model is important, in view of the unsteady problem which is ill-posed (see [5, 4]). There is a great analogy between the *steady* dispersion-reaction BOD/DO model and the steady stream-function/vorticity formulation of the incompressible fluid flow in the two-dimensional case, due to the non-symmetry of the boundary conditions on b and c

(see [7]). The main difference lies in the reaction terms in equations (1.1) which play a preponderous role. The fact that the related coefficients (r, r_*) are not equal arise tedious mathematical difficulties when they are non-constant. The stream-function/vorticity problem is a symmetric variational saddle point problem while the variational problem that follows from the BOD/DO model turns out to be non-symmetric. The corresponding theory originally developed by F. Brezzi (see [10]) applies to the former system while for the latter one, the generalized theory proposed in [19] (see also [6]) is better suited and therefore necessary for our purpose. The inf-sup statements required in the saddle point analysis turn out to be complicated. The results proven here are restricted to a class of reaction parameters, roughly characterized by the fact that the oscillations of the ratio r_*/r are bounded. Nevertheless, we do not consider this limitation as stringent since this assumption covers a wide part of the physical situations (see [17]).

Once the structure of system (1.1) is understood, we construct a first finite element discrete problem by the Galerkin method. But the same difficulties as for the stream-function/vorticity problem lead to a lack of convergence of its solution. So, following the approach in [2] and [3], we propose a modified problem where stabilization terms are added to overcome the previous difficulty. The a priori analysis is then performed for a wide class of reaction parameters (r, r_*) . The mixed finite element method we propose is proved to be optimal. Some numerical experiments confirm the interest of the stabilization, in good coherence with the analysis.

The outline of the paper is as follows:

- In Section 2, we write the variational formulation of problem (1.1) and prove its well-posedness.
- Section 3 is devoted to the description of the first finite element discrete problem.
- In Section 4, we introduce a stabilized finite element discrete problem and prove its well-posedness together with optimal a priori estimates.
- Numerical experiments leading to a comparison of the two discrete problems are presented in Section 5.
- Some concluding remarks are stated in Section 6.

FUNCTIONAL NOTATION. From now on, Ω is a bounded connected domain in \mathbb{R}^k , $k = 2$ or 3 , and its boundary $\partial\Omega$ is Lipschitz-continuous. The Lebesgue space of square integrable functions over Ω is denoted by $L^2(\Omega)$, and (\cdot, \cdot) is the associated scalar product. The Sobolev space $H^1(\Omega)$ contains all the functions that belong to $L^2(\Omega)$ so as their first-order derivatives. We also denote by $H_0^1(\Omega)$, the subspace of $H^1(\Omega)$ made of all functions whose traces on $\partial\Omega$ vanish (see [1]). The dual space of $H_0^1(\Omega)$ is $H^{-1}(\Omega)$ and the duality pairing is represented by $\langle \cdot, \cdot \rangle_{H^{-1}, H_0^1}$. The space $H^{1/2}(\partial\Omega)$ is the range of $H^1(\Omega)$ by the trace operator and $H^{-1/2}(\partial\Omega)$ is its dual space. We refer to [1] for more details on these functional spaces.

2 The mixed variational framework

From now on, we assume that the reaction and diffusion coefficients r , r_* and d are piecewise continuous on $\overline{\Omega}$ and also that there exist positive real constants r_b , r_\sharp , d_b and d_\sharp such that

$$\forall \mathbf{x} \in \overline{\Omega}, \quad r_b \leq r(\mathbf{x}), r_*(\mathbf{x}) \leq r_\sharp \quad \text{and} \quad d_b \leq d(\mathbf{x}) \leq d_\sharp. \quad (2.1)$$

We also suppose the diffusion coefficient d to be piecewise continuously differentiable on $\overline{\Omega}$. Some further regularity of the boundary and these coefficients is needed for some specific properties of problem (1.1), we assume them only when needed.

To develop our analysis we make a simplification assumption about the boundary data, that is $(\alpha, \beta) = (0, 0)$, and discuss the case of non-homogeneous boundary data only at the end of this section. We take the data f in $H^{-1}(\Omega)$ and g in $L^2(\Omega)$, respectively.

2.1 The variational formulation

The functional framework well fit to the system is the same as the one introduced in [7] (see also [8, Section II.4]) for the stream-function/vorticity formulation of the incompressible fluid flow. It has already been used in [5] for the organic pollution with constant reaction parameters. Before providing details, we need some further notation. Consider the functional space

$$\mathbb{V} = \left\{ \chi \in L^2(\Omega); \quad \operatorname{div}(d \nabla \chi) \in H^{-1}(\Omega) \right\}.$$

which is a Hilbert space when endowed with the graph norm

$$\|\chi\|_{\mathbb{V}} = \left(\|\operatorname{div}(d \nabla \chi)\|_{H^{-1}(\Omega)}^2 + \|\chi\|_{L^2(\Omega)}^2 \right)^{1/2}.$$

Observe that $H_0^1(\Omega)$ is a closed subspace of \mathbb{V} and that the norm $\|\cdot\|_{\mathbb{V}}$ is equivalent to $\|\cdot\|_{H^1(\Omega)}$ in $H_0^1(\Omega)$.

To write down the mixed variational formulation of problem (1.1), we multiply the first line in (1.1) by a function ψ in $H_0^1(\Omega)$. This leads to

$$\langle -\operatorname{div}(d \nabla b) + r b, \psi \rangle_{H^{-1}, H_0^1} = \langle f, \psi \rangle_{H^{-1}, H_0^1}.$$

Next, we multiply the second line in (1.1) by a function φ in \mathbb{V} , and using the duality yields that

$$\langle -\operatorname{div}(d \nabla \varphi) + r_* \varphi, c \rangle_{H^{-1}, H_0^1} + (r b, \varphi) = (g, \varphi).$$

To write the variational formulation of the system, let us introduce three bilinear forms,

$$\begin{aligned} \forall (\chi, \varphi) \in \mathbb{V} \times \mathbb{V}, \quad & a(\chi, \varphi) = (r \chi, \varphi), \\ \forall (\psi, \varphi) \in H_0^1(\Omega) \times \mathbb{V}, \quad & m(\psi, \varphi) = \langle -\operatorname{div}(d \nabla \varphi) + r \varphi, \psi \rangle_{H^{-1}, H_0^1}, \\ \forall (\psi, \varphi) \in H_0^1(\Omega) \times \mathbb{V}, \quad & m_*(\psi, \varphi) = \langle -\operatorname{div}(d \nabla \varphi) + r_* \varphi, \psi \rangle_{H^{-1}, H_0^1}, \end{aligned}$$

and also the linear form

$$\forall \varphi \in \mathbb{V}, \quad \ell(\varphi) = (g, \varphi).$$

All these forms are continuous on the spaces where they are defined.

The mixed variational problem may then be expressed in terms of these bilinear forms as follows:
Find (b, c) in $\mathbb{V} \times H_0^1(\Omega)$ fulfilling

$$\begin{aligned} \forall \psi \in H_0^1(\Omega), \quad m(\psi, b) &= \langle f, \psi \rangle_{H^{-1}, H_0^1}, \\ \forall \varphi \in \mathbb{V}, \quad m_*(c, \varphi) + a(b, \varphi) &= \ell(\varphi). \end{aligned} \quad (2.2)$$

The following equivalence property is easily derived from the arguments in [4, Lemma 2.1].

Lemma 2.1 *A pair (b, c) in $\mathbb{V} \times H_0^1(\Omega)$ is a solution of the mixed variational problem (2.2) if and only if it satisfies the boundary value system (1.1) with $\alpha = \beta = 0$.*

We recall that, according to the analysis of the abstract problem achieved in [19] and [8, Thm 1.3.14], necessary and sufficient conditions on the bilinear forms are required to ensure existence, uniqueness, and stability for the mixed problem (2.2). The bilinear form $a(\cdot, \cdot)$ must satisfy an inf-sup condition and a positivity property on both null-spaces of the forms $m(\cdot, \cdot)$ and $m_*(\cdot, \cdot)$; similar inf-sup conditions must also be satisfied by $m(\cdot, \cdot)$ and $m_*(\cdot, \cdot)$ in $H_0^1(\Omega) \times \mathbb{V}$.

2.2 The bilinear forms $m(\cdot, \cdot)$ and $m_*(\cdot, \cdot)$

The next results easily follow from the imbedding of $H_0^1(\Omega)$ into \mathbb{V} , see [5, Lemma 3.2] or [7, Section 2], and are derived by taking φ equal to ψ .

Lemma 2.2 *The bilinear form $m(\cdot, \cdot)$ satisfies the inf-sup condition on the space $H_0^1(\Omega) \times \mathbb{V}$, for a positive constant η only depending on r_b and d_b ,*

$$\forall \psi \in H_0^1(\Omega), \quad \sup_{\varphi \in \mathbb{V}} \frac{m(\psi, \varphi)}{\|\varphi\|_{\mathbb{V}}} \geq \eta \|\psi\|_{H^1(\Omega)}. \quad (2.3)$$

Lemma 2.3 *The bilinear form $m_*(\cdot, \cdot)$ satisfies the inf-sup condition on the space $H_0^1(\Omega) \times \mathbb{V}$, for a positive constant η_* only depending on r_b and d_b ,*

$$\forall \psi \in H_0^1(\Omega), \quad \sup_{\varphi \in \mathbb{V}} \frac{m_*(\psi, \varphi)}{\|\varphi\|_{\mathbb{V}}} \geq \eta_* \|\psi\|_{H^1(\Omega)}. \quad (2.4)$$

2.3 The bilinear form $a(\cdot, \cdot)$

The inf-sup conditions on $a(\cdot, \cdot)$ use the kernels of the bilinear forms $m(\cdot, \cdot)$ and $m_*(\cdot, \cdot)$ and require therefore their characterization. They are defined to be

$$\begin{aligned} \mathcal{N} &= \left\{ \varphi \in \mathbb{V}; \quad \forall \psi \in H_0^1(\Omega), \quad m(\psi, \varphi) = 0 \right\} \\ \mathcal{N}_* &= \left\{ \varphi \in \mathbb{V}; \quad \forall \psi \in H_0^1(\Omega), \quad m_*(\psi, \varphi) = 0 \right\}. \end{aligned}$$

The following statement is readily checked

$$\begin{aligned} \mathcal{N} &= \left\{ \varphi \in \mathbb{V}, \quad -\operatorname{div}(d \nabla \varphi) + r \varphi = 0 \text{ in } \Omega \right\}, \\ \mathcal{N}_* &= \left\{ \varphi \in \mathbb{V}, \quad -\operatorname{div}(d \nabla \varphi) + r_* \varphi = 0 \text{ in } \Omega \right\}. \end{aligned}$$

Note that \mathcal{N} and \mathcal{N}_* are closed subspaces in \mathbb{V} and are then Hilbert spaces, when endowed with $\|\cdot\|_{\mathbb{V}}$. Furthermore, the norm $\|\cdot\|_{L^2(\Omega)}$ is obviously equivalent to $\|\cdot\|_{\mathbb{V}}$ in both spaces \mathcal{N} and \mathcal{N}_* , where the constants of equivalence depend only on r_b and r_{\sharp} .

Remark 2.4 In the case $f = 0$, problem (2.2) turns out to be equivalent to the reduced one: *Find b in \mathcal{N} fulfilling*

$$\forall \varphi \in \mathcal{N}_*, \quad a(b, \varphi) = \ell(\varphi).$$

To solve this equation, one needs the couple of inf-sup conditions we look for.

The main purpose now is to bound from below the following inf-sup quantities

$$\inf_{\psi \in \mathcal{N}} \sup_{\varphi \in \mathcal{N}_*} \frac{a(\varphi, \psi)}{\|\varphi\|_{\mathbb{V}} \|\psi\|_{\mathbb{V}}} \quad \text{and} \quad \inf_{\psi \in \mathcal{N}_*} \sup_{\varphi \in \mathcal{N}} \frac{a(\varphi, \psi)}{\|\varphi\|_{\mathbb{V}} \|\psi\|_{\mathbb{V}}}.$$

This relies on the construction of a suitable isomorphism \mathcal{K} between \mathcal{N} and \mathcal{N}_* . To do this, for any χ in \mathcal{N} , we consider the solution θ in $H_0^1(\Omega)$ of the Poisson problem

$$-\operatorname{div}(d \nabla \theta) + r_* \theta = (r - r_*) \chi \quad \text{in } \Omega. \quad (2.5)$$

This elliptic boundary value problem is obviously well-posed. Then, we set: $\mathcal{K}\chi = \theta + \chi$. The function $\mathcal{K}\chi$ belongs to \mathcal{N}_* . The operator \mathcal{K} is then well-defined from \mathcal{N} into \mathcal{N}_* . Its properties are stated in the next lemma. For simplicity, we introduce the weighted norms defined by

$$\|\chi\|_{L_r^2(\Omega)} = (\chi, \chi r)^{1/2} \quad \text{and} \quad \|\varphi\|_{L_{r_*}^2(\Omega)} = (\varphi, \varphi r_*)^{1/2}.$$

Lemma 2.5 *The operator \mathcal{K} is an isomorphism between the spaces \mathcal{N} and \mathcal{N}_* . Moreover, the following inequalities hold*

$$\forall \chi \in \mathcal{N}, \quad \sigma_b \|\chi\|_{L^2(\Omega)} \leq \|\mathcal{K}\chi\|_{L^2(\Omega)} \leq \sigma_{\sharp} \|\chi\|_{L^2(\Omega)}, \quad (2.6)$$

for constants σ_b and σ_{\sharp} only depending on r_b and r_{\sharp} .

Proof. It is straightforward that equation (2.5) is equivalent to

$$-\operatorname{div}(d \nabla \theta) + r \theta = (r - r_*) \varphi \quad \text{in } \Omega. \quad (2.7)$$

With any function φ in \mathcal{N} , we associate the function $\varphi = \mathcal{K}\chi$ in \mathcal{N}_* . We have that $\mathcal{K}^{-1}\varphi = \varphi - \theta$, so that the inverse \mathcal{K}^{-1} of \mathcal{K} is well-defined.

To prove (2.6), with any χ in \mathcal{N} , we associate the function $\varphi = \mathcal{K}\chi = \theta + \chi$ in \mathcal{N}_* , where θ belongs to $H_0^1(\Omega)$ and satisfies equation (2.5). It is therefore easily derived that

$$\|\varphi\|_{L_{r_*}^2(\Omega)} = \|\theta + \chi\|_{L_{r_*}^2(\Omega)} \leq \varsigma_{\sharp} \|\chi\|_{L_r^2(\Omega)},$$

for a positive constant ς_{\sharp} only depending on the quantities r_{\sharp} and r_b introduced in (2.1). Exactly the same arguments, now relying on equation (2.7), yield

$$\|\chi\|_{L_r^2(\Omega)} = \|\varphi - \theta\|_{L_r^2(\Omega)} \leq \frac{1}{\varsigma_b} \|\varphi\|_{L_{r_*}^2(\Omega)},$$

for another positive constant ς_b . By using the equivalence of the norms $\|\cdot\|_{L_r^2(\Omega)}$ (resp. $\|\cdot\|_{L_{r_*}^2(\Omega)}$) and $\|\cdot\|_{L^2(\Omega)}$, we conclude the proof.

This lemma is of great help for establishing the inf-sup conditions on $a(\cdot, \cdot)$ for a class of reaction parameters. Let us introduce the assumption

$$\text{osc} \sqrt{\frac{r_*}{r}} = \max_{\mathbf{x} \in \overline{\Omega}} \sqrt{\frac{r_*}{r}(\mathbf{x})} - \min_{\mathbf{x} \in \overline{\Omega}} \sqrt{\frac{r_*}{r}(\mathbf{x})} < 2. \quad (2.8)$$

Before stating the inf-sup conditions, we need a further technical lemma. We skip its proof which is nearly obvious.

Lemma 2.6 *Let ρ be a piecewise continuous and positive function in $\overline{\Omega}$. There exists a positive real number ξ such that*

$$\forall \mathbf{x} \in \overline{\Omega}, \quad 1 - \frac{(\rho^2(\mathbf{x}) - \xi)^2}{4\rho^2(\mathbf{x})} \geq \zeta$$

for some $\zeta > 0$, if and only if

$$\text{osc} \rho = \max_{\mathbf{x} \in \overline{\Omega}} \rho(\mathbf{x}) - \min_{\mathbf{x} \in \overline{\Omega}} \rho(\mathbf{x}) < 2.$$

Lemma 2.7 *If assumption (2.8) holds, the bilinear form $a(\cdot, \cdot)$ satisfies the two inf-sup conditions, for a positive constant τ , only depending on r_b and r_\sharp ,*

$$\begin{aligned} \forall \chi \in \mathcal{N}, \quad \sup_{\varphi \in \mathcal{N}_*} \frac{a(\chi, \varphi)}{\|\varphi\|_{\mathbb{V}}} &\geq \tau \|\chi\|_{\mathbb{V}}, \\ \forall \varphi \in \mathcal{N}_*, \quad \sup_{\chi \in \mathcal{N}} \frac{a(\chi, \varphi)}{\|\chi\|_{\mathbb{V}}} &\geq \tau \|\varphi\|_{\mathbb{V}}. \end{aligned}$$

Proof. Let χ be given in \mathcal{N} , we associate $\varphi = \mathcal{K}\chi$ in \mathcal{N}_* . The function $\theta = \varphi - \chi$ belongs to $H_0^1(\Omega)$ and satisfies (2.5), or equivalently

$$-\text{div}(d \nabla \theta) + r_* \varphi - r \chi = 0 \quad \text{in } \Omega.$$

Multiplying this equation by θ and using Green's formula results in

$$\begin{aligned} \|\sqrt{d} \nabla \theta\|_{L^2(\Omega)^d}^2 + \|\varphi\|_{L_{r_*}^2(\Omega)}^2 + \|\chi\|_{L_r^2(\Omega)}^2 &= (r \chi, \varphi) + (r_* \chi, \varphi) \\ &= a(\chi, \varphi) + (r_* \chi, \varphi) = (1 + \xi) a(\chi, \varphi) + ((r_* - \xi r) \chi, \varphi), \end{aligned}$$

where ξ is some positive real number to be appropriately fixed later on. Owing to Young's inequality $ts \leq t^2 + s^2/4$, this formula yields

$$(1 + \xi) a(\chi, \varphi) + \|\varphi\|_{L_{r_*}^2(\Omega)}^2 + \left(\left[\frac{(r_* - \xi r)^2}{4rr_*} \right] r \chi, \chi \right) \geq \|\varphi\|_{L_{r_*}^2(\Omega)}^2 + \|\chi\|_{L_r^2(\Omega)}^2$$

whence

$$(1 + \xi) a(\chi, \varphi) \geq \int_{\Omega} r \chi^2(\mathbf{x}) \left[1 - \frac{(r_* - \xi r)^2}{4rr_*} \right] d\mathbf{x}.$$

Now, in view of assumption (2.8) and Lemma 2.6, the real number ξ may be selected such that

$$\min_{x \in \Omega} \left[1 - \frac{(r_* - \xi r)^2}{4rr_*} \right] = \zeta > 0. \quad (2.9)$$

Taking this bound into account yields that

$$\frac{a(\chi, \varphi)}{\|\chi\|_{L^2(\Omega)}} \geq c \frac{\zeta}{1 + \xi} \|\chi\|_{L^2(\Omega)} \geq c \frac{\zeta}{\sigma_{\#}(1 + \xi)} \|\varphi\|_{L^2(\Omega)} = \tau \|\varphi\|_{L^2(\Omega)}.$$

The first inf-sup condition is therefore proved since \mathcal{K} is an isomorphism and the norms $\|\cdot\|_{L^2(\Omega)}$ and $\|\cdot\|_{\mathbb{V}}$ are equivalent on the kernels \mathcal{N} and \mathcal{N}_* . The second one is checked following the same lines.

Remark 2.8 In the symmetric case where $r = r_*$, the forms $m(\cdot, \cdot)$ and $m_*(\cdot, \cdot)$ coincide, so that things are pretty easy. Indeed, the isomorphism \mathcal{K} reduces to the identity. As in the previous proof, choosing $\varphi = \mathcal{K}\chi = \chi$ gives that

$$a(\chi, \varphi) = \|\varphi\|_{L_r^2(\Omega)}^2.$$

A direct consequence is the proof of the inf-sup conditions on $a(\cdot, \cdot)$.

Remark 2.9 Despite the fact that we did not succeed in establishing both inf-sup conditions without assumption (2.8), we believe that this is only a technical problem and we suggest that it would be possible to prove that Lemma 2.7 holds without that assumption.

2.4 Existence and uniqueness

All the tools which are necessary and sufficient for the well-posedness of the mixed problem (2.2) are now available. We are hence in a position to state the main result of this section, which is straightforwardly derived from [6, Corollary 2.1] (see also [8, Thm 1.3.14]) and the generalized inf-sup conditions stated in Lemmas 2.2, 2.3 and 2.7.

Theorem 2.10 *Assume that (2.8) holds true. Then, for any data (f, g) in $H^{-1}(\Omega) \times L^2(\Omega)$, the mixed problem (2.2) has a unique solution (b, c) in $\mathbb{V} \times H_0^1(\Omega)$. Moreover this solution satisfies*

$$\|b\|_{\mathbb{V}} + \|c\|_{H^1(\Omega)} \leq C(\|f\|_{H^{-1}(\Omega)} + \|g\|_{L^2(\Omega)}). \quad (2.10)$$

2.5 Further regularity

We provide some indication about the “hidden” regularity of the solution (b, c) without investigating the issue in details. We then consider that the physical parameters d, r and r_* are constant. We put them all to unity, only for simplicity. The conclusions we make here are also valid for smooth space-varying coefficients. We begin with a basic result.

Lemma 2.11 *If the domain Ω is convex or has a boundary of class $\mathcal{C}^{1,1}$, the part c of the solution (b, c) of problem (1.1) belongs to $H^2(\Omega)$.*

Proof. The second and third lines of problem (1.1) in the case $\alpha = 0$ can be written as

$$\begin{aligned} -\Delta c + c &= g - b && \text{in } \Omega, \\ c &= 0 && \text{on } \partial\Omega. \end{aligned}$$

Due to the fact that $g - b$ belongs to $L^2(\Omega)$, we derive the desired result which follows from the elliptic regularity (see [14, Thms 2.4.2.5 & 3.2.1.2]).

Stating the regularity of the full solution (b, c) is more tricky and a further argument is needed.

Proposition 2.12 *Assume that the domain Ω is a convex polygon or polyhedron or has a boundary of class $\mathcal{C}^{1,1}$. For any data (f, g) in $H^{-1}(\Omega) \times H^1(\Omega)$, the solution (b, c) of problem (1.1) belongs to $H^1(\Omega) \times H^3(\Omega)$.*

Proof. Applying the Laplace operator to the second line in (1.1) yields the fourth order elliptic problem

$$\begin{aligned} -\Delta c + \Delta^2 c &= -\Delta g - f + b && \text{in } \Omega, \\ c = \partial_n c &= 0 && \text{on } \partial\Omega. \end{aligned}$$

The right-hand side of this equation belongs to $H^{-1}(\Omega)$. The regularity property of c is hence a consequence of [15, Cor. 3.4.2], according to the geometry of Ω . The regularity of b is then a direct consequence of the second line of (1.1).

2.6 Nonhomogeneous boundary conditions

Enforcing the nonhomogeneous boundary conditions on the boundary $\partial\Omega$ is worth some comments. In view of the functional framework used in our analysis, prescribing the Dirichlet condition $c = \alpha$ seems natural in $H^{1/2}(\partial\Omega)$ while imposing the Neumann one $d\partial_n c = \beta$ arises some trouble. The main difficulty for this problem is to derive its variational formulation. It reads as follows: *Find (b, c) in $\mathbb{V} \times H_0^1(\Omega)$ satisfying $c|_{\partial\Omega} = \alpha$ and*

$$\begin{aligned} \forall \psi \in H_0^1(\Omega), \quad m(\psi, b) &= \langle f, \psi \rangle_{H^{-1}, H_0^1}, \\ \forall \varphi \in \mathbb{V}, \quad m_*(c, \varphi) + a(b, \varphi) &= \ell(\varphi) - \langle \beta, \varphi \rangle_{\partial\Omega}. \end{aligned}$$

The point is that the duality product $\langle \beta, \varphi \rangle_{\partial\Omega}$ is meaningless for all φ in \mathbb{V} . To give a rigorous sense to it, we recall from [15, Section 1.5] that, if the boundary $\partial\Omega$ is smooth, any φ in \mathbb{V} has a trace $\varphi|_{\partial\Omega}$ that belongs to $H^{-1/2}(\partial\Omega)$. As a result for $\langle \beta, \varphi \rangle_{\partial\Omega}$ to make sense, it is necessary to assume that β lies in $H^{1/2}(\partial\Omega)$. This regularity seems too strong to consider on a Neumann data. This difficulty can be overcome by using an appropriate lifting and we have therefore the following result.

Theorem 2.13 *Assume that (2.8) holds true. Then, for any data (f, g) in $H^{-1}(\Omega) \times L^2(\Omega)$ and (α, β) in $H^{1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$, the boundary value system (1.1) has a unique solution (b, c) in $\mathbb{V} \times H^1(\Omega)$.*

Proof. Since the problem is linear, the uniqueness of its solution follows from the fact that the only solution for zero data is zero, which is a consequence of Lemma 2.1 and Theorem 2.10. On the other hand, the problem

$$\begin{aligned} -\operatorname{div}(d \nabla \bar{c}) + r_* \bar{c} &= 0 & \text{in } \Omega \\ d \partial_n \bar{c} &= \beta & \text{on } \partial\Omega, \end{aligned}$$

has a unique solution \bar{c} in $H^1(\Omega)$. Then, the same arguments as for Lemma 2.1 yield that (b, c) is a solution of problem (1.1) if and only if (b, c_0) , with $c_0 = c - \bar{c}$, is a solution in $\mathbb{V} \times H^1(\Omega)$ of

$$c_0 = \alpha - \bar{c} \quad \text{on } \partial\Omega,$$

and

$$\begin{aligned} \forall \psi \in H_0^1(\Omega), \quad m(\psi, b) &= \langle f, \psi \rangle_{H^{-1}, H_0^1}, \\ \forall \varphi \in \mathbb{V}, \quad m_*(c_0, \varphi) + a(b, \varphi) &= \ell(\varphi). \end{aligned}$$

Proving the existence of a solution to this problem is performed as for Theorem 2.10, whence the desired result.

Remark 2.14 When the boundary $\partial\Omega$ and the data (f, g) are smooth enough, the unknown b belongs to $H^1(\Omega)$, hence has a trace on $\partial\Omega$. Moreover, we can write, for any function ψ in $H^1(\Omega)$

$$\langle d \partial_n b, \psi \rangle = (\operatorname{div}(d \nabla b), \psi) + (d \nabla b, \nabla \psi),$$

which gives a sense to the BOD flux $d \partial_n b$. This is important, since even if these quantities do not appear in system (1.1), they have a physical meaning and computing them is of high interest.

3 A first finite element discrete problem

We aim to write a finite element discretization of the variational problem (2.2). The domain Ω is then assumed to be a polygon ($k = 2$) or a polyhedron ($k = 3$) to be splitted in a finite number of triangles or tetrahedra. We introduce a regular family $(\mathcal{T}_h)_h$ of triangulations of Ω , in the sense that, for each h ,

- $\bar{\Omega}$ is the union of all elements of \mathcal{T}_h ;
- The intersection of two different elements of \mathcal{T}_h , if not empty, is a vertex or a whole edge or a whole face of both of them;
- The ratio of the diameter h_K of any element K of \mathcal{T}_h to the diameter of its inscribed circle or sphere is smaller than a constant σ independent of h .

As usual, h stands for the maximum of the diameters h_K . We refer to [12, 9] for the basics of the finite element method.

The previous analysis of the continuous BOD-DO model illustrates the complication due by the lack of symmetry of the variational saddle point formulation. This is caused by the fact that the reaction parameters are different, and the same difficulty appears in the discrete case.

3.1 The discrete problem

We introduce the discrete spaces $\mathbb{V}_h \subset \mathbb{V}$ and $\mathbb{H}_h \subset H_0^1(\Omega)$, defined by

$$\mathbb{V}_h = \left\{ \chi_h \in H^1(\Omega); \quad \forall K \in \mathcal{T}_h, \quad (\chi_h)|_K \in \mathcal{P}_1(K) \right\}, \quad \mathbb{H}_h = \mathbb{V}_h \cap H_0^1(\Omega),$$

where $\mathcal{P}_1(K)$ stands for the space of restrictions to K of affine functions on \mathbb{R}^k . Using finite elements of degree higher than unity is allowed and the analysis in this case can be carried out similarly. Then, the first discrete problem in the case $\alpha = \beta = 0$ is constructed from (2.2) by the Ritz-Galerkin method. It reads as: *Find (b_h, c_h) in $\mathbb{V}_h \times \mathbb{H}_h$ fulfilling*

$$\begin{aligned} \forall \psi_h \in \mathbb{H}_h, \quad m_h(\psi_h, b_h) &= \langle f, \psi_h \rangle_{H^{-1}, H_0^1}, \\ \forall \varphi_h \in \mathbb{V}_h, \quad m_{*,h}(c_h, \varphi_h) + a(b_h, \varphi_h) &= \ell(\varphi_h), \end{aligned} \tag{3.1}$$

where the bilinear forms $m_h(\cdot, \cdot)$ and $m_{*,h}(\cdot, \cdot)$ are defined by

$$\begin{aligned} \forall (\psi_h, \varphi_h) \in \mathbb{H}_h \times \mathbb{V}_h, \quad m_h(\psi_h, \varphi_h) &= (d \nabla \varphi_h, \nabla \psi_h) + (r \varphi_h, \psi_h), \\ \forall (\psi_h, \varphi_h) \in \mathbb{H}_h \times \mathbb{V}_h, \quad m_{*,h}(\psi_h, \varphi_h) &= (d \nabla \varphi_h, \nabla \psi_h) + (r_* \varphi_h, \psi_h). \end{aligned}$$

Note that the new bilinear forms $m_h(\cdot, \cdot)$ and $m_{*,h}(\cdot, \cdot)$ coincide with $m(\cdot, \cdot)$ and $m_*(\cdot, \cdot)$, respectively, on $H_0^1(\Omega) \times H^1(\Omega)$, hence on $\mathbb{H}_h \times \mathbb{V}_h$.

Remark 3.1 Since \mathbb{H}_h is a closed subspace of $H_0^1(\Omega)$, for reasons already stated in Section 2, the norm $\|\cdot\|_{\mathbb{V}}$ is equivalent to $\|\cdot\|_{H^1(\Omega)}$ in \mathbb{H}_h .

Remark 3.2 When the coefficients r and r_* (and d) are too complex to be exactly taken into account in the practical computations, they are most often replaced by their Lagrange interpolates in \mathbb{V}_h . We do not consider this modification here because it only generates technicalities.

3.2 Existence and Uniqueness

Proving the well-posedness of the discrete problem (3.1) relies on the same arguments as for the continuous problem (2.2). Therefore, we need first some inf-sup conditions on the forms $m_h(\cdot, \cdot)$, and $m_{*,h}(\cdot, \cdot)$.

Lemma 3.3 *There exist two positive constants η' and η'_* independent of h such that the bilinear forms $m_h(\cdot, \cdot)$ and $m_{*,h}$ satisfy the discrete inf-sup conditions*

$$\begin{aligned} \forall \psi_h \in \mathbb{H}_h, \quad \sup_{\varphi_h \in \mathbb{V}_h} \frac{m_h(\psi_h, \varphi_h)}{\|\varphi_h\|_{\mathbb{V}}} &\geq \eta' \|\psi_h\|_{H^1(\Omega)}, \\ \forall \psi_h \in \mathbb{H}_h, \quad \sup_{\varphi_h \in \mathbb{V}_h} \frac{m_{*,h}(\psi_h, \varphi_h)}{\|\varphi_h\|_{\mathbb{V}}} &\geq \eta'_* \|\psi_h\|_{H^1(\Omega)}. \end{aligned}$$

Proof. For any ψ_h in \mathbb{H}_h , taking φ_h equal to ψ_h yields

$$m_h(\psi_h, \varphi_h) \geq c \|\psi_h\|_{H^1(\Omega)}^2 = c \|\psi_h\|_{H^1(\Omega)} \|\varphi_h\|_{H^1(\Omega)} \geq \eta' \|\psi_h\|_{H^1(\Omega)} \|\varphi_h\|_{\mathbb{V}}.$$

This and the same argument applied to $m_{*,h}(\cdot, \cdot)$ yield the desired result.

Proving the required inf-sup conditions on the bilinear form $a(\cdot, \cdot)$ requires more work. We first introduce the discrete kernels

$$\begin{aligned} \mathcal{N}_h &= \left\{ \varphi_h \in \mathbb{V}_h; \quad \forall \psi_h \in \mathbb{H}_h, \quad m_h(\psi_h, \varphi_h) = 0 \right\}, \\ \mathcal{N}_{*,h} &= \left\{ \varphi_h \in \mathbb{V}_h; \quad \forall \psi_h \in \mathbb{H}_h, \quad m_{*,h}(\psi_h, \varphi_h) = 0 \right\}. \end{aligned}$$

Note that \mathcal{N}_h is not a subspace of \mathcal{N} nor $\mathcal{N}_{*,h}$ is included in \mathcal{N}_* . As for the continuous problem, the bilinear form $a(\cdot, \cdot)$ should satisfy some inf-sup conditions on these subspaces and as for the continuous case we need the construction of an isomorphism \mathcal{K}_h between \mathcal{N}_h and $\mathcal{N}_{*,h}$. To do this, with any χ_h in \mathcal{N}_h , we associate the solution θ_h in \mathbb{H}_h of the problem

$$\forall \psi_h \in \mathbb{H}_h, \quad (d \nabla \theta_h, \nabla \psi_h) + (r_* \theta_h, \psi_h) = ((r - r_*) \chi_h, \psi_h). \quad (3.2)$$

This problem is well-posed, which enables us to set $\mathcal{K}_h \chi_h = \theta_h + \chi_h$. The operator \mathcal{K}_h is one-to-one from \mathcal{N}_h onto $\mathcal{N}_{*,h}$ and satisfies the following result.

Lemma 3.4 *There exist positive constants σ'_b and σ'_\sharp independent of h such that the following inequalities hold*

$$\forall \chi_h \in \mathcal{N}_h, \quad \sigma'_b \|\chi_h\|_{L^2(\Omega)} \leq \|\mathcal{K}_h \chi_h\|_{L^2(\Omega)} \leq \sigma'_\sharp \|\chi_h\|_{L^2(\Omega)}.$$

Proof. The second inequality follows by taking ψ_h equal to θ_h in problem (3.2), noting that $|\nabla \theta_h|_{H^1(\Omega)}$ is nonnegative, and using the inequality

$$\|\mathcal{K}_h \chi_h\|_{L^2(\Omega)} \leq \|\chi_h\|_{L^2(\Omega)} + \|\theta_h\|_{L^2(\Omega)}.$$

The first inequality is derived by the same arguments when noting that problem (3.2) is equivalent to (with obvious notation)

$$\forall \psi_h \in \mathbb{H}_h, \quad (d \nabla \theta_h, \nabla \psi_h) + (r \theta_h, \psi_h) = ((r - r_*) \varphi_h, \psi_h).$$

The proof is complete.

The inf-sup conditions on $a(\cdot, \cdot)$, restricted to $\mathbb{V}_h \times \mathbb{H}_h$ can be obtained following the same arguments as for the continuous problem. They require the Assumption (2.8) to be fulfilled.

Lemma 3.5 *Assume that (2.8) holds true. The bilinear form $a(\cdot, \cdot)$ satisfies the two inf-sup conditions, for a positive constant τ' independent of h ,*

$$\begin{aligned} \forall \chi_h \in \mathcal{N}_h, \quad \sup_{\varphi_h \in \mathcal{N}_{*,h}} \frac{a(\chi_h, \varphi_h)}{\|\varphi_h\|_{L^2(\Omega)}} &\geq \tau' \|\chi_h\|_{L^2(\Omega)}, \\ \forall \varphi_h \in \mathcal{N}_{*,h}, \quad \sup_{\chi_h \in \mathcal{N}_h} \frac{a(\chi_h, \varphi_h)}{\|\chi_h\|_{L^2(\Omega)}} &\geq \tau' \|\varphi_h\|_{L^2(\Omega)}. \end{aligned}$$

These last inf-sup conditions do not involve the right norm of the functions, which should be $\|\cdot\|_{H^1(\Omega)}$. However, since all norms are equivalent on the finite-dimensional spaces \mathcal{N}_h and $\mathcal{N}_{*,h}$, the well-posedness of problem (3.1) is a direct consequence of the previous results, see once more [6, Corollary 2.1] or [8, Thm 1.3.14].

Theorem 3.6 *Assume that (2.8) holds true. For any data (f, g) in $H^{-1}(\Omega) \times L^2(\Omega)$, the discrete problem (3.1) has a unique solution (b_h, c_h) in $\mathbb{V}_h \times \mathbb{H}_h$.*

Due to the weak norms in both inf-sup conditions of Lemma 3.5, a stability estimate analogous to (2.10) would involve constants depending on h . For the same reasons, the a priori error estimates that can be proved for this problem do not lead to the convergence of the solution for the discrete problem in all cases.

4 The stabilized discrete problem and its a priori analysis

A possible remedy to the difficulties encountered in the previous section, is to resort to the stabilized finite element discretization studied for the symmetric saddle point problems in [3]. The extension of this procedure to our non-symmetric problems arises some heavy technicalities. From now on and only for brevity of proofs, we take the coefficient d equal to 1.

4.1 The stabilized discrete problem

Let \mathcal{E}_h be the set of all edges ($k = 2$) or faces ($k = 3$) of elements of \mathcal{T}_h which are not contained in $\partial\Omega$. For each e in \mathcal{E}_h , we denote by h_e the diameter of e and by $[\cdot]_e$ the jump through e . The stabilized discrete problem relies on the same discrete spaces as previously, it now reads: *Find* (b_h, c_h) in $\mathbb{V}_h \times \mathbb{H}_h$ fulfilling

$$\begin{aligned} \forall \psi_h \in \mathbb{H}_h, \quad m_h(\psi_h, b_h) &= \langle f, \psi_h \rangle_{H^{-1}, H_0^1}, \\ \forall \varphi_h \in \mathbb{V}_h, \quad m_{*,h}(c_h, \varphi_h) + a_{\rho,h}(b_h, \varphi_h) &= \ell(\varphi_h), \end{aligned} \quad (4.1)$$

where the new bilinear form $a_{\rho,h}(\cdot, \cdot)$ is defined by

$$a_{\rho,h}(\chi_h, \varphi_h) = a(\chi_h, \varphi_h) + \rho \sum_{e \in \mathcal{E}_h} h_e \int_e [\partial_n \chi_h]_e(\tau) [\partial_n \varphi_h]_e(\tau) d\tau.$$

ρ is a positive real number called regularization parameter. We refer to [3] (see also [2]) for the introduction of this new form for the stream-function and vorticity formulation of the Stokes problem.

Remark 4.1 Observe that the bilinear form $a_{\rho,h}(\cdot, \cdot)$ is symmetric and positive-definite on \mathbb{V}_h . It is elliptic with respect to the L^2 -norm. Things are harder when we are involved in the natural norm of \mathbb{V} . This issue is investigated in the subsequent.

Remark 4.2 Handling high variations of the dispersion parameter $d = d(\mathbf{x})$ is made by modifying the augmented part of the stabilized bilinear form $a_{\rho,h}(\cdot, \cdot)$. It is then transformed into

$$\begin{aligned} a_{\rho,h}(\chi_h, \varphi_h) &= a(\chi_h, \varphi_h) + \rho \sum_{e \in \mathcal{E}_h} h_e \int_e [d \partial_n \chi_h]_e(\tau) [d \partial_n \varphi_h]_e(\tau) d\tau \\ &\quad + \rho \sum_{K \in \mathcal{T}_h} \text{meas}(K) \int_K \text{div}(d \nabla \chi_h) \text{div}(d \nabla \varphi_h) d\mathbf{x}. \end{aligned}$$

The overall analysis we undertake here is readily extended to this case, at the cost of more technical work, especially caused by the last term.

4.2 Well-posedness for the stabilized problem

Proving the existence, uniqueness and stability for the new discrete problem requires some preliminary lemmas which state several important properties of the augmented bilinear form $a_{\rho,h}(\cdot, \cdot)$, more precisely of the stabilizing form $s_h(\cdot, \cdot)$ defined by

$$s_h(\chi_h, \varphi_h) = \sum_{e \in \mathcal{E}_h} h_e \int_e [\partial_n \chi_h]_e(\tau) [\partial_n \varphi_h]_e(\tau) d\tau.$$

We begin with a result proven in [3, Proposition 6].

Lemma 4.3 *There exists a positive constant μ independent of h such that*

$$\forall \chi_h \in \mathbb{V}_h, \quad \sqrt{s_h(\chi_h, \chi_h)} \leq \mu \|\Delta \chi_h\|_{H^{-1}(\Omega)}.$$

The next lemmas provide the “inverse” inequality on the kernel spaces \mathcal{N}_h and $\mathcal{N}_{*,h}$. The proof is an adaptation of the one made for Proposition 7 in [3].

Lemma 4.4 *There exists a positive constant μ' independent of h such that*

$$\begin{aligned} \forall \chi_h \in \mathcal{N}_h, \quad \|\Delta \chi_h\|_{H^{-1}(\Omega)} &\leq \mu' \sqrt{a_{1,h}(\chi_h, \chi_h)}, \\ \forall \chi_h \in \mathcal{N}_{*,h}, \quad \|\Delta \chi_h\|_{H^{-1}(\Omega)} &\leq \mu' \sqrt{a_{1,h}(\chi_h, \chi_h)}. \end{aligned}$$

Proof. We handle the first estimate. The second one can be established following the same lines. Let $\chi_h \in \mathcal{N}_h$ be given. Then, for all $\psi \in H_0^1(\Omega)$ and $\psi_h \in \mathbb{H}_h$, we have that

$$(\nabla \chi_h, \nabla \psi) = (\nabla \chi_h, \nabla(\psi - \psi_h)) - (\chi_h, \psi_h r).$$

Making an integration by part and using the Cauchy-Schwarz inequality provide

$$\begin{aligned} (\nabla \chi_h, \nabla \psi) &= \sum_{e \in \mathcal{E}_h} \int_e [\partial_n \chi_h]_e(\tau)(\psi - \psi_h)(\tau) d\tau - (\chi_h, \psi_h r) \\ &\leq \sqrt{s_h(\chi_h, \chi_h)} \left(\sum_{e \in \mathcal{E}_h} (h_e)^{-1} \|\psi - \psi_h\|_{L^2(e)}^2 \right)^{1/2} - (\chi_h, \psi_h r). \end{aligned}$$

A suitable choice of ψ_h , equal to the Clément interpolant of ψ , the Bramble-Hilbert argument together with the Poincaré inequality yield that

$$(\nabla \chi_h, \nabla \psi) \leq \kappa \left(\sqrt{s_h(\chi_h, \chi_h)} |\psi|_{H^1(\Omega)} + \|\chi_h\|_{L_r^2(\Omega)} \|\psi\|_{L_r^2(\Omega)} \right) \leq \mu' \sqrt{a_{1,h}(\chi_h, \chi_h)} |\psi|_{H^1(\Omega)}.$$

By taking into account the identity

$$\|\Delta \chi_h\|_{H^{-1}(\Omega)} = \sup_{\psi \in H_0^1(\Omega)} \frac{1}{|\psi|_{H^1(\Omega)}} (\nabla \chi_h, \nabla \psi),$$

the proof is complete.

Corollary 4.5 *The map*

$$\chi_h \mapsto \sqrt{a_{\rho,h}(\chi_h, \chi_h)}$$

is a norm on \mathcal{N}_h (resp. $\mathcal{N}_{,h}$) that is equivalent to the norm of \mathbb{V} , uniformly in h (in the sense that the equivalence constants are independent of h).*

We will need also a third intermediary result, related to a bound of the bilinear form $s_h(\cdot, \cdot)$ by the H^1 -norm.

Lemma 4.6 *There exists a positive constant μ'' independent of h such that*

$$\forall \chi_h \in \mathbb{V}_h, \quad s_h(\chi_h, \chi_h) \leq \mu'' |\chi_h|_{H^1(\Omega)}^2.$$

Proof. Let χ_h belong to \mathbb{V}_h . Denoting by K and K' the two elements of \mathcal{T}_h that share e , we have straightforwardly

$$h_e \int_e [\partial_n \chi_h]_e^2(\tau) d\tau \leq h_e |(\nabla \chi_h)|_K|_{L^2(e)^k}^2 + h_e |(\nabla \chi_h)|_{K'}|_{L^2(e)^k}^2.$$

Switching backward and forward to the reference element, provides the following bound

$$h_e \int_e [\partial_n \chi_h]_e^2(\tau) d\tau \leq \kappa (|(\chi_h)|_K|_{H^1(K)}^2 + |(\chi_h)|_{K'}|_{H^1(K')}^2),$$

where the constant κ depends on the regularity parameter of the family of triangulations. Summing up over e , we derive that

$$\sum_{e \in \mathcal{E}_h} h_e \int_e [\partial_n \chi_h]_e^2(\tau) d\tau \leq \mu'' |\chi_h|_{H^1(\Omega)}^2.$$

The proof is complete.

A first consequence of Lemma 4.3 is that the bilinear form $a_{\rho,h}(\cdot, \cdot)$ is continuous on $\mathbb{V}_h \times \mathbb{V}_h$ with respect to the natural norm $\|\cdot\|_{\mathbb{V}}$. The continuity constant is bounded independently of h .

Proposition 4.7 *There exists a positive constant C_ρ independent of h such that*

$$\forall (\chi_h, \varphi_h) \in \mathbb{V}_h \times \mathbb{V}_h, \quad a_{\rho,h}(\chi_h, \varphi_h) \leq C_\rho \|\chi_h\|_{\mathbb{V}} \|\varphi_h\|_{\mathbb{V}}.$$

Proof. Let χ_h and φ_h be in \mathbb{V}_h . By Cauchy-Schwarz inequality, there holds that

$$\begin{aligned} a_{\rho,h}(\chi_h, \varphi_h) &= a(\chi_h, \varphi_h) + \rho s_h(\chi_h, \varphi_h) \\ &\leq \|\chi_h\|_{L_T^2(\Omega)} \|\varphi_h\|_{L_T^2(\Omega)} + \rho \sqrt{s_h(\chi_h, \chi_h)} \sqrt{s_h(\varphi_h, \varphi_h)}. \end{aligned}$$

Invoking the result of Lemma 4.3 gives

$$a_{\rho,h}(\chi_h, \varphi_h) \leq \|\chi_h\|_{L_T^2(\Omega)} \|\varphi_h\|_{L_T^2(\Omega)} + \mu^2 \rho \|\Delta \chi_h\|_{H^{-1}(\Omega)} \|\Delta \varphi_h\|_{H^{-1}(\Omega)}.$$

This yields that

$$a_{\rho,h}(\chi_h, \varphi_h) \leq C \max(1, \rho) \|\chi_h\|_{\mathbb{V}} \|\varphi_h\|_{\mathbb{V}}.$$

The proof is complete with $C_\rho = C \max(1, \rho)$.

Now, proving the desired inf-sup conditions for the augmented bilinear form $a_{\rho,h}(\cdot, \cdot)$ on the kernel spaces \mathcal{N}_h and $\mathcal{N}_{*,h}$, with respect to the norm of \mathbb{V} requires additional technical work. Let us first state the following lemma.

Lemma 4.8 Assume that (2.8) holds true. There exists a positive constant ρ_0 such that, for any $\rho \leq \rho_0$, the following positivity property holds

$$\forall \chi_h \in \mathcal{N}_h, \quad a_{\rho,h}(\chi_h, \mathcal{K}_h \chi_h) \geq \lambda \sqrt{a_{\rho,h}(\chi_h, \chi_h)} \sqrt{a_{\rho,h}(\mathcal{K}_h \chi_h, \mathcal{K}_h \chi_h)},$$

where the constant λ is positive and only depends on the reaction parameters (r, r_*) .

Proof. Let χ_h be given in \mathcal{N}_h . Thus, the function $\varphi_h = \mathcal{K}_h \chi_h$ belongs to $\mathcal{N}_{*,h}$, while the function $\theta_h = \varphi_h - \chi_h$ is the solution of problem (3.2). Processing as in the proof of Lemma 2.7 we are allowed to assert that, for some $\xi > 0$, we have

$$|\nabla \theta_h|_{H^1(\Omega)}^2 + \|\varphi_h\|_{L_{r_*}^2(\Omega)}^2 + \|\chi_h\|_{L_r^2(\Omega)}^2 = (1 + \xi)a(\chi_h, \varphi_h) + ((r_* - \xi r) \chi_h, \varphi_h),$$

Then, given the identity

$$-s_h(\theta_h, \theta_h) + s_h(\chi_h, \chi_h) + s_h(\varphi_h, \varphi_h) = 2s_h(\chi_h, \varphi_h),$$

we derive that

$$\begin{aligned} |\nabla \theta_h|_{H^1(\Omega)}^2 - \frac{1}{2}(1 + \xi)\rho s_h(\theta_h, \theta_h) + \frac{1}{2}(1 + \xi)\rho s_h(\chi_h, \chi_h) \\ + \frac{1}{2}(1 + \xi)\rho s_h(\varphi_h, \varphi_h) + \|\varphi_h\|_{L_{r_*}^2(\Omega)}^2 + \|\chi_h\|_{L_r^2(\Omega)}^2 = (1 + \xi)a(\chi_h, \varphi_h) \\ + (1 + \xi)\rho s_h(\chi_h, \varphi_h) + ((r_* - \xi r) \chi_h, \varphi_h). \end{aligned}$$

Using Lemma 4.6 yields that

$$\begin{aligned} \left(1 - \frac{1}{2}(1 + \xi)\rho \mu''\right) |\theta_h|_{H^1(\Omega)}^2 + \frac{1}{2}(1 + \xi)\rho s_h(\chi_h, \chi_h) + \frac{1}{2}(1 + \xi)\rho s_h(\varphi_h, \varphi_h) \\ + \|\varphi_h\|_{L_{r_*}^2(\Omega)}^2 + \|\chi_h\|_{L_r^2(\Omega)}^2 \leq (1 + \xi) a_{\rho,h}(\chi_h, \varphi_h) + ((r_* - \xi r) \chi_h, \varphi_h). \end{aligned}$$

Recall that $a_{\rho,h}(\cdot, \cdot) = a(\cdot, \cdot) + \rho s_h(\cdot, \cdot)$. Due to assumption (2.8), it is possible to select ξ as in (2.9). This results in

$$\begin{aligned} (1 + \xi) a_{\rho,h}(\chi_h, \varphi_h) \geq \left(1 - \frac{1}{2}(1 + \xi)\rho \mu''\right) |\theta_h|_{H^1(\Omega)}^2 \\ + \frac{1}{2}(1 + \xi)\rho s_h(\chi_h, \chi_h) + \frac{1}{2}(1 + \xi)\rho s_h(\varphi_h, \varphi_h) + \varsigma \|\chi_h\|_{L_r^2(\Omega)}^2 \end{aligned}$$

(note that ς depends on r and r_*). Applying now Lemma 3.4, we get

$$\begin{aligned} (1 + \xi) a_{\rho,h}(\chi_h, \varphi_h) \geq \left(1 - \frac{1}{2}(1 + \xi)\rho \mu''\right) |\theta_h|_{H^1(\Omega)}^2 \\ + \frac{1}{2}(1 + \xi)\rho s_h(\chi_h, \chi_h) + \frac{1}{2}(1 + \xi)\rho s_h(\varphi_h, \varphi_h) + \varsigma \|\chi_h\|_{L_r^2(\Omega)}^2 + \varsigma \|\varphi_h\|_{L_{r_*}^2(\Omega)}^2. \end{aligned}$$

The constant ς is positive and does not depend neither on ρ nor on h . It is only sensitive to the reaction parameters (r, r_*) . Next, if ρ is small enough, then the coefficient of $|\theta_h|_{H^1(\Omega)}^2$ is nonnegative and can be dropped without changing the inequality. Hence, we obtain

$$\begin{aligned} (1 + \xi) a_{\rho,h}(\chi_h, \varphi_h) \geq \frac{1}{2}(1 + \xi)\rho s_h(\chi_h, \chi_h) + \varsigma \|\chi_h\|_{L_r^2(\Omega)}^2 \\ + \frac{1}{2}(1 + \xi)\rho s_h(\varphi_h, \varphi_h) + \varsigma \|\varphi_h\|_{L_{r_*}^2(\Omega)}^2. \end{aligned}$$

This bound can be put under the following form

$$a_{\rho,h}(\chi_h, \varphi_h) \geq \frac{\lambda}{2} \left(a_{\rho,h}(\chi_h, \chi_h) + a_{\rho,h}(\varphi_h, \varphi_h) \right),$$

for a constant $\lambda > 0$ that is dependent on (ξ, ς) (which are themselves dependent on (r, r_*)). Next, thanks to the positive definiteness of $a_{\rho,h}(\cdot, \cdot)$, we finally obtain

$$a_{\rho,h}(\chi_h, \varphi_h) \geq \lambda \sqrt{a_{\rho,h}(\chi_h, \chi_h)} \sqrt{a_{\rho,h}(\varphi_h, \varphi_h)}.$$

The proof is complete.

Remark 4.9 The following bound holds true

$$\forall \varphi_h \in \mathcal{N}_{*,h}, \quad a_{\rho,h}((\mathcal{K}_h)^{-1} \varphi_h, \varphi_h) \geq \lambda \sqrt{a_{\rho,h}((\mathcal{K}_h)^{-1} \varphi_h, (\mathcal{K}_h)^{-1} \varphi_h)} \sqrt{a_{\rho,h}(\varphi_h, \varphi_h)}.$$

We are now in position to state the inf-sup conditions satisfied by $a_{\rho,h}(\cdot, \cdot)$ on the kernel spaces \mathcal{N}_h and $\mathcal{N}_{*,h}$.

Proposition 4.10 *Assume that the regularization parameter ρ is sufficiently small. Then, when (2.8) holds true, the following inf-sup conditions on $a_{\rho,h}(\cdot, \cdot)$ are satisfied*

$$\begin{aligned} \forall \chi_h \in \mathcal{N}_h, \quad \sup_{\varphi_h \in \mathcal{N}_{*,h}} \frac{a_{\rho,h}(\chi_h, \varphi_h)}{\|\varphi_h\|_{\mathbb{V}}} &\geq \tau_\rho \|\chi_h\|_{\mathbb{V}}, \\ \forall \varphi_h \in \mathcal{N}_{*,h}, \quad \sup_{\chi_h \in \mathcal{N}_h} \frac{a_{\rho,h}(\chi_h, \varphi_h)}{\|\chi_h\|_{\mathbb{V}}} &\geq \tau_\rho \|\varphi_h\|_{\mathbb{V}}. \end{aligned}$$

The inf-sup constant τ_ρ is expected to decay to zero when ρ decreases toward zero.

Proof. Let χ_h be given in \mathcal{N}_h and denote $\varphi_h = \mathcal{K}_h \chi_h \in \mathcal{N}_{*,h}$. By Lemma 4.8, we derive

$$\frac{a_{\rho,h}(\chi_h, \varphi_h)}{\|\varphi_h\|_{\mathbb{V}}} \geq \lambda \sqrt{a_{\rho,h}(\chi_h, \chi_h)} \frac{\sqrt{a_{\rho,h}(\varphi_h, \varphi_h)}}{\|\varphi_h\|_{\mathbb{V}}}.$$

Now, applying Corollary 4.5 yields that

$$\begin{aligned} \frac{a_{\rho,h}(\chi_h, \varphi_h)}{\|\varphi_h\|_{\mathbb{V}}} &\geq \lambda \sqrt{a_{\rho,h}(\chi_h, \chi_h)} \frac{\sqrt{a_{\rho,h}(\varphi_h, \varphi_h)}}{\sqrt{a_{1,h}(\varphi_h, \varphi_h)}} \\ &\geq \lambda (\min(1, \sqrt{\rho}))^2 \sqrt{a_{1,h}(\chi_h, \chi_h)} \geq c \lambda \min(1, \rho) \|\chi_h\|_{\mathbb{V}}. \end{aligned}$$

The constant τ_ρ may be equal to $\lambda \rho$ for small values of ρ . The second inf-sup condition can be established similarly using Remark 4.9 instead of Lemma 4.8. The proof is complete.

The following existence and uniqueness theorem is now a direct consequence of Lemma 3.3 and Propositions 4.7 and 4.10.

Theorem 4.11 *Assume that (2.8) holds true and that ρ is small enough. For any data (f, g) in $H^{-1}(\Omega) \times L^2(\Omega)$, the stabilized discrete problem (4.1) has a unique solution (b_h, c_h) in $\mathbb{V}_h \times \mathbb{H}_h$. The following stability holds*

$$\|b_h\|_{\mathbb{V}} + \|c_h\|_{H^1(\Omega)} \leq C_\rho (\|f\|_{H^{-1}(\Omega)} + \|g\|_{L^2(\Omega)}). \quad (4.2)$$

The constant C_ρ is expected to blow up when ρ decays to zero.

4.3 A priori error estimates

From now on, we always assume that condition (2.8) holds true and that ρ is small enough, in order that the discrete problem (4.1) is well-posed. We now prove an a priori error estimate between the solutions (b, c) of problem (2.2) and (b_h, c_h) of problem (4.1). As usual, we introduce the affine subspace

$$\mathcal{N}_h(f) = \left\{ \varphi_h \in \mathbb{V}_h; \quad \forall \psi_h \in \mathbb{H}_h, \quad m_h(\psi_h, \varphi_h) = \langle f, \psi_h \rangle_{H^{-1}, H_0^1} \right\}.$$

The following lemma relies on standard arguments, but takes into account the stabilization of the form $a(\cdot, \cdot)$. It involves the norm $\|\cdot\|_*$ defined by

$$\|v\|_* = \left(\sum_{K \in \mathcal{T}_h} h_K \|v\|_{H^{\frac{3}{2}}(K)}^2 \right)^{\frac{1}{2}}.$$

Lemma 4.12 *Assume that the part b of the solution (b, c) of problem (2.2) belongs to $H^{3/2}(\Omega)$. The following a priori error estimate holds*

$$\|b - b_h\|_{\mathbb{V}} \leq \left(1 + \frac{C}{\tau_\rho}\right) \inf_{\beta_h \in \mathcal{N}_h(f)} (\|b - \beta_h\|_{\mathbb{V}} + \|b - \beta_h\|_*) + \frac{C}{\tau_\rho} \inf_{\gamma_h \in \mathbb{H}_h} \|c - \gamma_h\|_{H^1(\Omega)}.$$

Proof. Let β_h be any approximation of b in $\mathcal{N}_h(f)$. Thus, it follows from the first line in (4.1) that the function $b_h - \beta_h$ belongs to \mathcal{N}_h . Applying the first inf-sup condition in Proposition 4.10 yields

$$\|b_h - \beta_h\|_{\mathbb{V}} \leq \tau_\rho^{-1} \sup_{\varphi_h \in \mathcal{N}_{*,h}} \frac{a_{\rho,h}(b_h - \beta_h, \varphi_h)}{\|\varphi_h\|_{\mathbb{V}}}. \quad (4.3)$$

To evaluate the quantity $a_{\rho,h}(b_h - \beta_h, \varphi_h)$, we observe by using problem (4.1) that

$$a_{\rho,h}(b_h - \beta_h, \varphi_h) = \ell(\varphi_h) - m_{*,h}(c_h, \varphi_h) - a_{\rho,h}(\beta_h, \varphi_h).$$

Due to (2.2) together with the coincidence of the forms $m_*(\cdot, \cdot)$ and $m_{*,h}$ on the discrete spaces, we derive that

$$a_{\rho,h}(b_h - \beta_h, \varphi_h) = a(b - \beta_h, \varphi_h) + m_*(c - c_h, \varphi_h) - \rho s_h(\beta_h, \varphi_h).$$

Since φ_h belongs to $\mathcal{N}_{*,h}$ we have for all γ_h in \mathbb{H}_h

$$m_*(c - c_h, \varphi_h) = m_*(c - \gamma_h, \varphi_h).$$

On the other hand, because of the regularity of the solution b inside Ω , we derive

$$-s_h(\beta_h, \varphi_h) = s_h(b - \beta_h, \varphi_h).$$

The fact that $\mathbf{grad} b$ belongs to $L^2(\Omega)^k$ and that its divergence belongs to $L^2(\Omega)$ implies that each $[\partial_n b]_e$ belongs to $H^{-1/2}(e)$. Moreover, by an interpolation argument and since b belongs to $H^{3/2}(\Omega)$, then the flux jump $[\partial_n b]_e$ turns to be in $L^2(e)$. Combining this with a standard inequality on φ_h give

$$-s_h(\beta_h, \varphi_h) \leq \sum_{e \in \mathcal{E}_h} h_e \|[\partial_n(b - \beta_h)]\|_{L^2(e)} \|[\partial_n \varphi_h]\|_{L^2(e)} \leq C \|b - \beta_h\|_* \|\varphi_h\|_{\mathbb{V}}.$$

Inserting all this into (4.3) gives

$$\|b_h - \beta_h\|_{\mathbb{V}} \leq \frac{C}{\tau_\rho} (\|b - \beta_h\|_{\mathbb{V}} + \|c - \gamma_h\|_{H^1(\Omega)} + \|b - \beta_h\|_*).$$

We conclude the proof by using a triangle inequality.

The next lemma is now just an extension of [13, Chap. II, eq. (1.16)].

Lemma 4.13 *If the assumptions of Lemma 4.12 are satisfied, the following bound holds*

$$\inf_{\beta_h \in \mathcal{N}_h(f)} (\|b - \beta_h\|_{\mathbb{V}} + \|b - \beta_h\|_*) \leq C \inf_{\beta_h \in \mathbb{V}_h} (\|b - \beta_h\|_{\mathbb{V}} + \|b - \beta_h\|_*).$$

Proof. For any function β_h in \mathbb{V}_h , we deduce from the continuity and ellipticity of the form $m_h(\cdot, \cdot)$ on \mathbb{H}_h that there exists a function η_h in \mathbb{H}_h which satisfies

$$\forall \psi_h \in \mathbb{H}_h, \quad m_h(\psi_h, \eta_h) = \langle f, \psi_h \rangle_{H^{-1}, H_0^1} - m_h(\psi_h, \beta_h) = m(\psi_h, b) - m_h(\psi_h, \beta_h).$$

Thus the function $\tilde{\beta}_h = \beta_h + \eta_h$ belongs to $\mathcal{N}_h(f)$ and estimating the norm of $b - \tilde{\beta}_h$ follows from a triangle inequality, the previous equation and a local inverse inequality applied to η_h .

Finally, we evaluate the error on the part c_h of the solution.

Lemma 4.14 *If the assumptions of Lemma 4.12 are satisfied, the following a priori error estimate holds*

$$\|c - c_h\|_{H^1(\Omega)} \leq C \left(\|b - b_h\|_{\mathbb{V}} + \inf_{\gamma_h \in \mathbb{H}_h} \|c - \gamma_h\|_{H^1(\Omega)} + \inf_{\beta_h \in \mathbb{V}_h} (\|b - \beta_h\|_{\mathbb{V}} + \|b - \beta_h\|_*) \right).$$

Proof. From the second inf-sup condition in Lemma 3.3, it suffices to evaluate the quantity, for any φ_h in \mathbb{V}_h ,

$$m_{*,h}(c_h - \gamma_h, \varphi_h) = m_*(c - \gamma_h, \varphi_h) + a(b - b_h, \varphi_h) - \rho s_h(b_h, \varphi_h).$$

Bounding the first two terms simply follows from Cauchy-Schwarz inequalities. To estimate the last one, we note that

$$-s_h(b_h, \varphi_h) = s_h(b - b_h, \varphi_h) = s_h(b - \beta_h, \varphi_h) + s_h(\beta_h - b_h, \varphi_h),$$

use the same arguments as in the proof of Lemma 4.12 for the first quantity, Lemma 4.3 and a triangle inequality for the last one. This gives the desired result.

We are now in a position to state explicit error estimates. The proof follows from Lemmas 4.12, 4.13 and 4.14, together with the approximation properties of the spaces \mathbb{V}_h and \mathbb{H}_h and an interpolation argument for handling nonsmooth solutions (b, c) .

Theorem 4.15 *Assume that the solution (b, c) of problem (2.2) belongs to the space $H^{r+1}(\Omega) \times H^{s+1}(\Omega)$, $0 \leq r, s \leq 1$. The following a priori error estimates hold*

$$\|b - b_h\|_{\mathbb{V}} + \|c - c_h\|_{H^1(\Omega)} \leq C_\rho \left(h^r \|b\|_{H^{r+1}(\Omega)} + h^s \|c\|_{H^{s+1}(\Omega)} \right).$$

The constant C_ρ is expected to blow up when ρ decays to zero.

Remark 4.16 These estimates are fully optimal with respect to h . Furthermore, when combined with the stability property (4.2), they yield the convergence of (b_h, c_h) towards (b, c) when h tends to zero, for any fixed parameter ρ .

5 Numerical experiments

Computations are realized by means of the code **FreeFem++** developed by F. Hecht (see [16]), where a script specifically dedicated to the pollution system is made.

We wish to compare the two discrete problems, which we call in the following NS (for non stabilized) and S (for stabilized), in a basic case. The domain is the square

$$\Omega =]-\frac{1}{2\pi}, -\frac{1}{2\pi} + 1]^2.$$

Both Neumann and Dirichlet conditions are enforced on c , and b is free of any boundary condition. The exact solution, represented in Figure 5.1, is given by

$$b(x_1, x_2) = \cos\left(\frac{3\pi}{2}x_1\right) \cos\left(\frac{3\pi}{2}x_2\right), \quad c(x_1, x_2) = \sin\left(\frac{3\pi}{2}x_1\right) \sin\left(\frac{3\pi}{2}x_2\right).$$

The dispersion and reaction parameters are constant and fixed to $d = 0.151$ and $(r, r_*) = (0.2, 0.4)$. According to some specialized literature, they are close to real-life values. For reasons explained later on, we also consider this same solution in the disk with centre $(0, 0)$ and radius $1/2$, computed with the same coefficients.

Figure 5.1 represents, from top to bottom, the exact solution and the solution issued from NS. For the non stabilized problem, we can see in this figure that the error on b is stronger than the error on c ; this error is concentrated on the corners of the domain. To check that this is due to the discretization and not to the geometry of the domain, we now work with the domain Ω equal to the ball. Figure 5.2 represents the solution (b_h, c_h) of the NS problem. The degradation of the accuracy at the vicinity of the boundary is obvious. Thus, the NS problem does not lead to the convergence of the solution, as appears in the next figure.

In all the numerical simulations, the meshes are triangular and structured. Varying the mesh size on the square, we evaluate the errors on the BOD density b and the DO concentration c , with respect to the $H^1(\Omega)$ and $L^2(\Omega)$ norms, for both non-stabilized and stabilized approximations. The related convergence curves are plotted in Figure 5.3 in logarithmic scales.

- For the NS problem, there is no convergence of b_h in the $H^1(\Omega)$ -norm, and the slope in the $L^2(\Omega)$ -norm is evaluated to 1.09. This is an indication of the necessity to resort to stabilization. On the other hand, the slopes of the convergence curves for c in the $(H^1(\Omega), L^2(\Omega))$ norms are close to $(0.99, 1.99)$.
- For the S problem, the slopes for c are close to the previous ones, equal to $(0.99, 1.88)$. However, the slopes for b are now equal to $(1.28, 1.67)$, so that the convergence for b is highly improved.

Finally, in order to illustrate the good convergence properties of the stabilized problem, Figure 5.4 represent the solutions b_h and c_h issued from S, first for a standard mesh ($h = \frac{1}{48}$), second for a refined mesh ($h = \frac{1}{96}$).

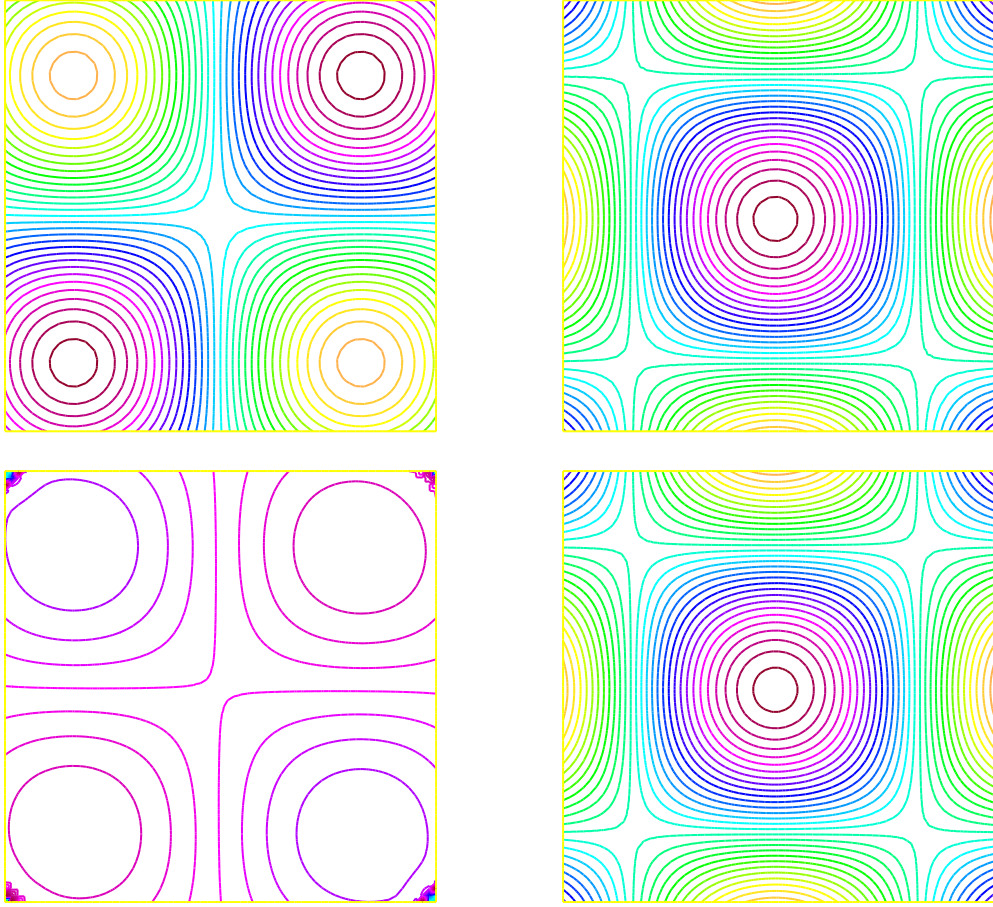


Figure 5.1: Exact and NS computed solutions, b and b_h in the left panels, c and c_h in the right panels.

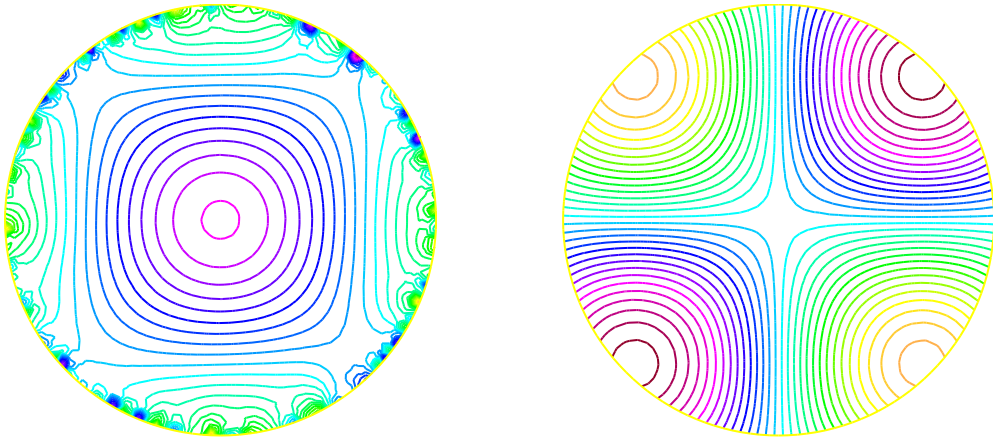


Figure 5.2: NS Computed solutions in the disk, b_h in the left panel, c_h in the right panel.

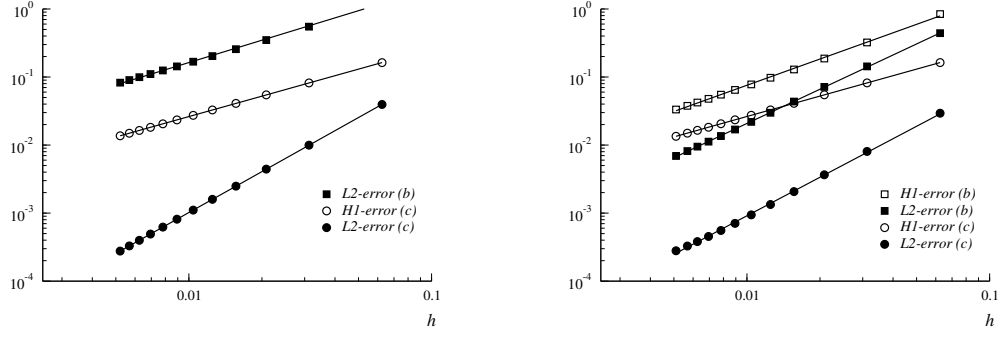


Figure 5.3: Convergence curves for the $H^1(\Omega)$ and $L^2(\Omega)$ norms, for both NS (left) and S (right) problems.

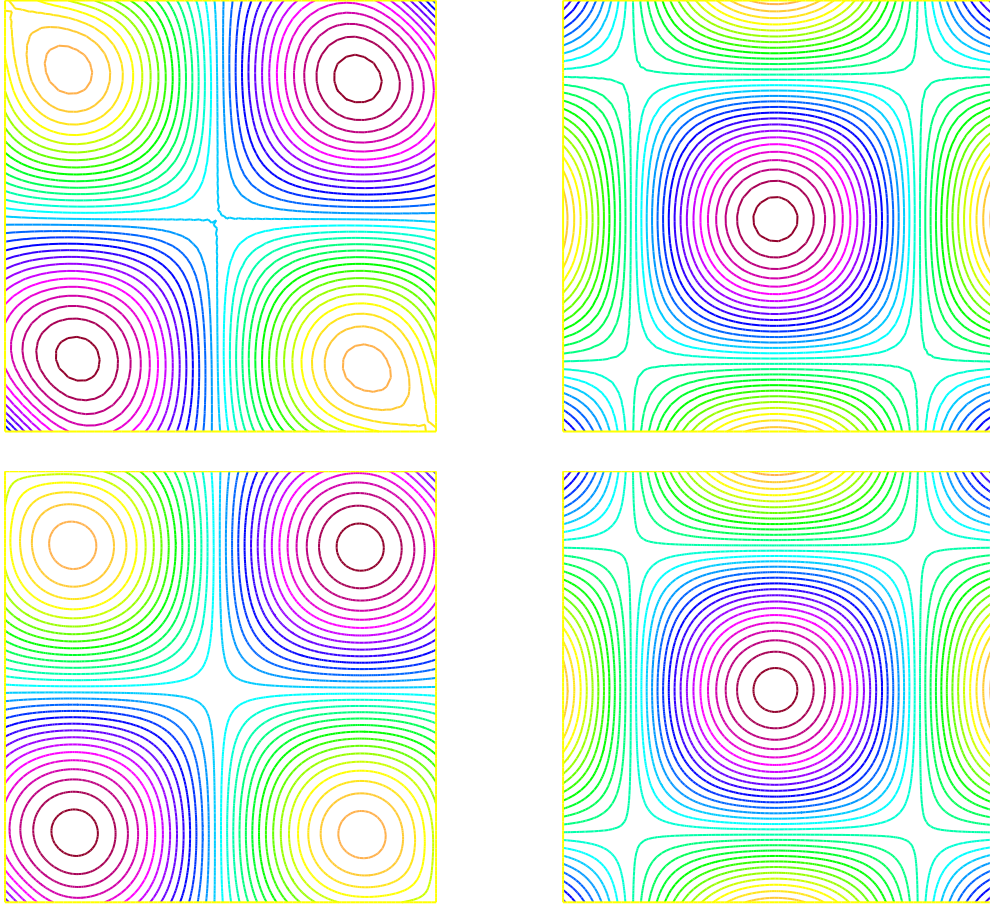


Figure 5.4: S computed solutions, b_h in the left panels, c_h in the right panels, on different meshes.

6 Conclusion

The steady pollution model studied here may be considered as a generalization of the well known saddle-point stream-function/vorticity $\psi - \omega$ problem used in the simulation of *two-dimensional* steady Stokes fluid flows (see [3, 8]). The difference between the two models resides in facts that first the pollution system is valid in three dimensions and second that it is non-symmetric with an additional reaction term with space dependent kinetics. This, unexpectedly, brings tedious complications in the analysis of the exact and discretized versions of it. From the applied mathematics view, this stirs a renewed interest (we may even speak of a rehabilitation) in the technical and numerical work realized so-far on the mixed stream-function/vorticity formulation of the Stokes model. Somehow the road is pathed for studying the pollution model, the questions to solve, the methodology to follow so as the ideas already developed may be reinvested or recast for the pollution model with however substantially increased mathematical difficulties to handle. They are successfully solved in this work. The short-term continuation is to deal with the a posteriori issues. We are currently investigating residual based error estimations and the stated results together with a deeper numerical experimentation will be exposed in the second part of this paper. A more distant goal is to consider the full unsteady pollution model which differs tremendously of the unsteady $\psi - \omega$ system. They are opposite in nature, the time-dependent pollution model turns out to be ill-posed (see [5]). Its space time discretization is expected to arise higher difficulties and requires some specific mathematical tools to pick up in the community inverse and ill-posed problems. We refer to the Ph.-D. thesis [18] to have some clues on these issues and on close ones but also to discover several applications of the unsteady pollution modes, especially in the inverse problem of (polluting) source detection and identification.

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